Data Evaluation Report on the aerobic biotransformation of oxyfluorfen in water-sediment system

PMRA Submission Number {.....} EPA MRID Number 46373104

Data Requirement: PMRA Data Code:
EPA DP Barcode: D312066
OECD Data Point:
EPA Guideline: 162-4

Test material:

Common name:	Oxyfluorfen.
Chemical name:	
IUPAC name:	2-Chloro-α,α,α-trifluoro-p-tolyl -3-ethoxy-4-nitrophenyl ether.
CAS name:	2-Chloro-1-(3-ethoxy-4-nitrophenoxy)-4-(trifluoromethyl)benzene.
CAS No.:	42874-03-3.
Synonyms	RH-2915; Goal.
Smiles string:	FC(c1ccc(c(c1)Cl)Oc1ccc(c(c1)OCC)N(=O)=O)(F)F (ISIS v2.3/Universal SMILES). Clc1cc(C(F)(F)F)ccc1Oc2cc(OCC)c(N(=O)(=O))cc2 (EPI Suite, v3.12).

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CITATION: Mamouni, A. 2002. [^{14}C]-Oxyfluorfen: route and rate of degradation in aquatic systems. Unpublished study performed by RCC Ltd., Itingen, Switzerland; sponsored and submitted by DOW AgroSciences LLC, Indianapolis, IN. RCC Study Number 827190. Experiment initiated March 26, 2002, and completed December 09, 2002 (p. 12). Final report issued December 20, 2002.

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EXECUTIVE SUMMARY:

The aerobic biotransformation of [chlorophenyl-U-^{14}C]-labeled 2-chloro-α,α,α-trifluoro-p-tolyl-3-ethoxy-4-nitrophenyl ether (oxyfluorfen) was studied in a river water/sandy loam sediment system (water pH 8.24, dissolved organic carbon not reported; sediment pH 7.47, organic carbon 1.1%) and in a pond water/silt loam sediment system (water pH 8.08, dissolved organic carbon not reported; sediment pH 7.17, organic carbon 2.5%) each from Switzerland for 100 days in dark at 20 ±2°C. [^{14}C]Oxyfluorfen was applied at a nominal rate of 0.480 mg a.i./L to both test systems. The water:sediment ratios used were *ca.* 5:1 for the river water/sandy loam sediment system and *ca.* 8:1 for the pond water/silt loam sediment system. The experiment was conducted in accordance with the USEPA Subdivision IV, Section 162-4, and in compliance with OECD and Swiss Good Laboratory Practices. The test system consisted of glass flasks (1 L) containing water (550 mL) and sediment (220 g wet) that were incubated for *ca.* 1 month prior to treatment; during this time, air was drawn through the flask headspace and the water layer was gently agitated from above with a suspended magnetic stirrer. Following treatment, the flasks were attached to a volatile trapping system for the collection of CO_2 and organic volatile compounds. Moistened air was drawn through a sample, then sequentially through ethylene glycol and 2N NaOH solutions. Duplicate samples were analyzed after 0, 0.25, 1, 2, 7, 14, 28, 56, and 100 days of incubation. The water layer was removed by pipette and mixed with acetonitrile, and aliquots were analyzed using LSC. The sediment was extracted three times with acetonitrile:water (8:2, v:v) at room temperature, and samples collected at and after 7 days posttreatment were Soxhlet-extracted with acetonitrile:water (8:2, v:v); extracts were analyzed for total radioactivity using LSC. The water and the sediment extracts were partitioned with ethyl acetate, and aliquots of the aqueous and organic phases were analyzed using LSC. The organic phases and any aqueous phases that contained >5% of the applied were concentrated and analyzed for total radioactivity using LSC and for [^{14}C]oxyfluorfen and its transformation products using HPLC. Oxyfluorfen was identified by comparison to an unlabeled reference standard; no reference standards for transformation products were identified. Identifications were confirmed using TLC. Portions of the extracted soil were analyzed for total radioactivity using LSC following combustion. Extracted soil from samples collected at 100 days was further extracted with acetonitrile:1.0N HCl (1:1, v:v; harsh extraction), and unextracted residues were fractionated into fulvic acid, humic acid, and humin. Volatile traps were analyzed for total radioactivity using LSC.

The incubation temperature (20 ± 2EC) was maintained throughout the experiment; no supporting data were provided. The pH of the river water averaged 8.27 ± 0.21 and of the pond water averaged 8.15 ± 0.11. During the study, oxic conditions were maintained in the water and anoxic conditions in the sediment; the redox potentials in the river water ranged from 172 to 220mV, and in the sediment ranged from -98 to -161 mV. Redox potentials in the pond water ranged from 157 to 322 mV and in the sediment ranged from -73 to -151 mV.

Overall recoveries of [^{14}C]residues averaged 93.9 ± 3.6% (range 86.4-100.8%) of the applied from the river system and 94.9 ±2.7% (90.9-101.6%) from the pond system. The ratio of

[^{14}C]residues in the water and sediment was *ca.* 2:1 (v:w) at 0.25 days posttreatment, 1:1 at 2 days, 1:4 at 7 days, and 1:10 at 56 days.

In the total **river water/sediment system** (water plus sediment), oxyfluorfen dissipated with a half-life of 47 days based on first order linear regression analysis and 40 days based on nonlinear regression (single, 2 parameter) analysis. [^{14}C]Oxyfluorfen varied from an average of 93.0 to 98.4% of the applied at 0 through 2 days posttreatment with no pattern of decline, then decreased to 85.5-86.3% at 7 and 14 days, 47.2% at 28 days, and 25.3% % at 100 days (study termination). In the water and sediment, oxyfluorfen dissipated with linear half-lives of 11.6 and 61.9 days, respectively, and nonlinear half-lives of 4.7 and 50.6 days, respectively. In the water, [^{14}C]oxyfluorfen averaged 62.2-68.6% of the applied at 0-0.25 days posttreatment, then decreased to 15.8-19.8% at 7 and 14 days, 4.0% at 28 days and <0.3% at 100 days. In the sediment, [^{14}C]oxyfluorfen increased to a maximum average of 70.5% of the applied at 7 days posttreatment, then decreased to 32.9% at 56 days and 25.2% at 100 days. No major transformation products were isolated during the study. Six minor transformation products (M2, M3, M5, M6, M7, M8) were isolated. These compounds were not identified; they were not detected until 14 days posttreatment and each averaged ≤4.9% of the applied through 100 days with one exception. M5 was 9.6% of the applied in one sample at 28 days posttreatment; M5 was not detected in the replicate sample from this interval and averaged 3.7% at 100 days.

In the river sediment, total extractable [^{14}C]residues increased to a maximum average of 70.6% of the applied at 7 days posttreatment, then declined to 31.8% at 100 days, while nonextractable [^{14}C]residues increased to a maximum of 45.6% at 100 days. Harsh extraction of the 100-day extracted sediment released an additional 6.8-7.1% of the applied, which consisted of at least two very polar compounds. Fractionation of the nonextracted residues in the 100-day harsh-extracted soil (36.2-41.0% of the applied) determined that 2.3-2.5%, 0.6-0.7%, and 33.3-37.8% of the applied was associated with fulvic acids, humic acids, and humin, respectively. At study termination (100 days), $^{14}CO_2$ and volatile organic [^{14}C]residues totaled an average 9.0% and 0.5% of the applied, respectively.

In the total **pond water/sediment system**, oxyfluorfen dissipated with a half-life of 27 days based on first order linear regression analysis and 30 days based on nonlinear regression (single, 2 parameter) analysis. [^{14}C]Oxyfluorfen varied from an average of 92.8 to 99.0% at 0 through 2 days posttreatment with no pattern of decline, then decreased to 85.0% at 7 days, 51.2% at 28 days, 25.6% at 56 days, and 7.9% at 100 days (study termination). In the water and sediment, oxyfluorfen dissipated with linear half-lives of 10.8 and 28.3 days, respectively, and nonlinear half-lives of 3.9 and 31.5 days, respectively. In the water, [^{14}C]oxyfluorfen averaged 53.9-71.4% of the applied at 0-1 day posttreatment, then decreased to 16.9% at 7 days, 5.9% at 14 days and 2.6% at 56 days (last interval analyzed). In the sediment, [^{14}C]oxyfluorfen increased to a maximum average of 68.1% of the applied at 7 days posttreatment, then decreased to 23.0% at 56 days and 7.9% at 100 days. No major transformation products were isolated during the study. Eight minor transformation products (M1, M2, M3, M4, M5, M6, M7, M9) were isolated. These

compounds were not identified; they were not detected until 14 days posttreatment and each averaged ≤3.5% of the applied through 100 days.

In the pond sediment, total extractable [^{14}C]residues increased to a maximum average of 68.1% of the applied at 7 days posttreatment, then declined to 24.9% at 100 days, while nonextractable [^{14}C]residues increased to a maximum of 59.3% at 100 days. Harsh extraction of the 100-day extracted sediment released an additional 15.5-17.2% of the applied, which consisted of at least two very polar compounds. Fractionation of the nonextracted residues in the 100-day harsh-extracted soil (42.6-43.3% of the applied) determined that 1.7-2.0%, 2.7-2.8%, and 38.2-38.5% of the applied was associated with fulvic acids, humic acids, and humin, respectively. At study termination (100 days), $^{14}CO_2$ and volatile organic [^{14}C]residues totaled an average 9.4% and 0.8% of the applied, respectively, in the pond system.

A transformation pathway was provided by the study author. Oxyfluorfen applied to water dissipates rapidly by mineralization to CO_2 and minor transformation products and by incorporated into the organic matter of the sediment.

Results Synopsis:

Test system used: River water/sandy loam sediment
Half-life/DT50 in water:
- Linear half-life: 11.6 days (r^2 = 0.9222).
- Non-linear half-life: 4.7 days (r^2 = 0.9538).
- Observed DT50: <7 days.

Half-life/DT50 in sediment:
- Linear half-life: 61.9 days (r^2 = 0.8131).
- Non-linear half-life: 50.6 days (r^2 = 0.9792).
- Observed DT50: *ca.* 56 days.

Half-life/DT50 in total system:
- Linear half-life: 47.2 days (r^2 = 0.8815).
- Non-linear half-life: 39.6 days (r^2 = 0.9248).
- Observed DT50: *ca.* 28 days.

Major transformation products:
- None.

Minor transformation products:
- CO_2.
- Other minor transformation products (six) were not identified.

Test system used: Pond water/silt loam sediment
Half-life/DT50 in water:
- Linear half-life: 10.8 days (r^2 = 0.7686).
- Non-linear half-life: 3.9 days (r^2 = 0.9584).
- Observed DT50: <7 days.

Half-life/DT50 in sediment:
- Linear half-life: 28.3 days (r^2 = 0.9286).
- Non-linear half-life: 31.5 days (r^2 = 0.9858).
- Observed DT50: <56 days.

Half-life/DT50 in total system:
- Linear half-life: 26.9 days (r^2 = 0.9573).
- Non-linear half-life: 29.6 days (r^2 = 0.9797).
- Observed DT50: *ca.* 28 days.

Major transformation products:
- CO_2.

Minor transformation products:
- Minor transformation products (eight) were not identified.

Study Acceptability: This study is classified as **supplemental** and scientifically valid. The study was conducted under gradient redox potential with water under oxic conditions and sediment under anoxic conditions. In addition, it could not be determined if the foreign soils used in this study are comparable to soils found in a typical oxyfluorfen use area in the United States. Also, an aerobic aquatic metabolism study using a soil from the US may be requested.

I. MATERIALS AND METHODS

GUIDELINE FOLLOWED: This study was conducted in accordance with the USEPA Subdivision IV, Section 162-4 (1982); OECD Draft Guideline "Aerobic-Anaerobic Transformation in Water Sediment Systems" (1999); Commission Directive 95/36/EC (1995); and SETAC Part 8, 8.2- aerobic aquatic degradation (1995; p. 15). One significant deviation from the objectives of USEPA Subdivision N Guidelines was noted:

> A soil from the US was not studied, and it could not be determined if the foreign soils that were used in the study were typical of the pesticide use area in the US. This does not affect the validity of the study.

COMPLIANCE: This study was conducted in compliance with OECD and Swiss Good Laboratory Practices (pp. 3-3a; Appendix 2, p. 87). Signed and dated Data Confidentiality, GLP, and Quality Assurance statements were provided (pp. 2-3a, 5-6). A Certificate of Authenticity was not provided.

A. MATERIALS:

1. Test Material [Chlorophenyl ring-UL-^{14}C]oxyfluorfen (RH-2915; p. 18).

Chemical Structure: See DER Attachment 1.

Description: Technical grade.

Purity: Radiochemical purity: 100% (by HPLC, p. 18).
Lot/Batch No. 734.01.
RCC No. 116856/A.
Analytical purity: Not reported.
Specific activity: 22.39 mCi/g (0.8296 MBq/mg).
Locations of the radiolabel: Uniformly labeled in the chlorophenyl ring.

Storage conditions of test chemicals: The radiolabeled test substance was stored in the dark at *ca.* -20°C (p. 18). The unlabeled test substance was stored at room temperature (p. 17).

Physico-chemical properties of oxyfluorfen:

Parameter	Value	Comment
Molecular weight	361.7 g/mole.	
Molecular formula	$C_{15}H_{11}ClF_3NO_4$	
Water Solubility	0.116 mg/L.	At 25EC.
Organic solubility	72.5 g/100 g.	In acetone at 25EC.
Vapor Pressure/Volatility	Not reported.	
UV Absorption	Not reported.	
Pka	Not reported.	
K_{ow}/log K_{ow}	Not reported.	
Stability of compound at room temperature, if provided	Decomposed readily by UV radiation; DT50 = 3 days at room temperature.	

Data obtained from p. 17 of the study report.

2. Water collection, storage and properties

Table 1: Description of water collection and storage.

Description		River	Pond
Geographic location		Rhine (Rheinsulz AG/Switzerland) (47E32' N, 7E48' E)	Pond (Fr schiweiher BL/Switzerland) (47E33' N, 8E05' E)
Pesticide use history at the collection site		Not reported.	
Collection procedures for:	Water:	Not reported.	
	Sediment:	Not reported.	
Sampling depth for:	Water:	10-30 cm	
	Sediment:	0-5 cm	
Storage conditions		Stored in sealed containers at *ca.* 4EC.	
Storage length		*Ca.* 1 month.	
Preparation of water and sediment samples		Sediments were sieved (2 mm) and waters were filtered (0.2 mm) prior to use.	

Data were obtained from p. 19 of the study report.

Table 2: Properties of the water.

Description		River		Pond	
Temperature (°C)	Surface	6.5		8.5	
	5 cm above sediment	6.5		8.2	
pH	Surface	8.25		8.08	
	5 cm above sediment	8.24		8.08	
Redox potential (mv)		Initial	Final	Initial	Final
	Surface	245	127	233	131
	5 cm above sediment	241	133	234	136
Oxygen concentration (mg/L)	Surface	14.4		11.8	
	5 cm above sediment	14.6		11.7	
Dissolved organic carbon (%)		Not reported.		Not reported.	
Hardness (EdH)		16.5		24.5	
Electrical conductivity		Not reported.		Not reported.	
Biomass (mg microbial C/100 g or CFU or other)		Not reported.		Not reported.	

Data were obtained from Table 1, p. 41 of the study report.

Table 3: Properties of the sediment.

Property	River	Pond
Soil texture (USDA)	Sandy loam	Silt loam
% Sand (>0.05 mm)	58.4	25.9
% Silt (0.002-0.05 mm)	29.3	50.3
% Clay (<0.002 mm)	12.3	23.8
pH ($CaCl_2$)	7.47	7.17
Organic carbon (%)	1.1	2.5
CEC (mVal equivalents/100g dry sediment)	10.6	21.3
Redox potential (mV)	-167	-149
Bulk density (g/cm^3)	Not reported.	Not reported.
Biomass at the start of preincubation (mg microbial C/100 g)	61.2	134.8

Data were obtained from Table 2, p. 42 of the study report.

B. EXPERIMENTAL DESIGN:

1. Preliminary experiments: No preliminary experiments were reported.

2. Experimental conditions:

Table 4: Study design.

Parameter		River	Pond
Duration of the test		100 days following treatment.	
Water: Filtered/unfiltered water: Type and size of filter used, if any:		 Filtered. 0.2 mm sieve.	
Amount of sediment and water/ treatment		137 g dry wt (220 g wet) to 550 mL water	84 g dry wt. (220 g wet) to 550 mL water
Water/sediment ratio		4.6:1	8.2:1
Test concentrations: (mg a.i./L)	Nominal:	0.480 mg a.i./L.	
	Actual:	0.491 mg a.i./L (270 Φg a.i./550 mL water) or 0.480 mg a.i./L (264 Φg a.i./550 mL water) for the 6-hour samples.	
Control conditions, if used		Sterile controls were not used.	
No. of Replications	Controls	Sterile controls were not used.	
	Treatment	Two samples were collected at each sampling interval.	

Parameter		River		Pond	
Test apparatus (Type/material/volume)		Glass *ca.* 1 L flasks (*ca.* 10.6 cm i.d.) containing water (550 mL) and sediment (220 g wet wt) and incubated in the dark at 20 ∀ 2EC for *ca.* 1 month prior to treatment. During acclimation, the flasks were ventilated with moistened air and the water layers were gently agitated by stirring with a "suspended" magnetic stirrer. The samples were then treated and the flasks attached to a flow-through volatile trapping system. The flasks were incubated in the dark at 20 ∀ 2EC; the water layer was agitated during incubation. The test apparatus is illustrated in Scheme 3, p. 60.		
Details of traps for CO_2 and organic volatile, if any		Moistened air was pulled through a sample flask (30 mL/minute), then through one bottle of 50 mL ethylene glycol and one bottle of 50 mL 2N NaOH.		
If no traps were used, is the system closed?		Volatile traps were used.		
Identity and concentration of co-solvent		Acetone, *ca.* 0.07% by volume (0.40 mL/550 mL water) or *ca.* 0.06% by volume (0.35 mL/550 mL water) for the 6-hour samples.		
Test material application method	Volume of the test solution used/treatment:	400 ΦL/sample (350 ΦL/sample for the 6-hour samples).		
	Application method (eg: mixed/not mixed):	Test solution was applied dropwise to the water surface using a Hamilton syringe.		
Any indication of the test material adsorbing to the walls of the test apparatus?		Not reported.		
Microbial biomass/microbial population of the control		Sterile controls were not used in this study.		
Microbial biomass of the treated soil (mg C/100 g soil):	Water	Not determined.		
	Sediment	0 days	100 days	0 days	100 days
		50.2	41.2	132.7	103.4
Experimental conditions:	Temperature (°C):	20 ∀ 2		
	Continuous darkness (Yes/No):	Yes		
Other details, if any		None.		

Data were obtained from pp. 19-20, 22-23 and Table 2, p. 42 of the study report.

3. Aerobic conditions: To equilibrate the system and establish aerobic conditions, the sediment was flooded and incubated under an air atmosphere for *ca.* 1 month prior to treatment and the water layer was continuously stirred using a suspended magnetic stirrer (pp. 20, 23). After treatment, the test systems were incubated under continuous-flow (30 mL/minute) humidified air with the water being stirred for the duration of the study. The redox potential of the water and sediment of control samples, and the oxygen content of the water were measured at each sampling interval (Table 4, p. 44).

4. Supplementary experiments: No supplementary experiments were reported.

5. Sampling:

Table 5: Sampling details.

Criteria	Details
Sampling intervals	0, 0.25, 1, 2, 7, 14, 28, 56, and 100 days.
Sampling method	Two flasks of each system were collected at each interval.
Method of collection of CO_2 and organic volatile compounds	Trapping solutions were collected and replaced at each sampling interval and at 22 and 63 days.
Sampling intervals/times for: Sterility check: pH measurement: Redox potential/other:	 No sterile controls were used. Measured at each sampling interval. Measured at each sampling interval.
Sample storage before analysis	Samples were processed and analyzed immediately after sampling.
Other observation, if any	None.

Data were obtained from p. 23 and Tables 5-6, pp. 45-46 of the study report.

C. ANALYTICAL METHODS:

Separation of the sediment and water: The water and sediment were separated using a pipette (p. 24; Scheme 1, p. 58). Residual water in the sediment was treated as sediment in further analyses.

Extraction/clean up/concentration methods for water and sediment samples: To increase the solubility of oxyfluorfen, the water was mixed with acetonitrile (20%, v:v; p. 24; Scheme 1, p. 58). Aliquots were analyzed using LSC. The water (100 mL) was partitioned twice with ethyl acetate (2 x 50 mL), aliquots of the aqueous and organic phases were analyzed using LSC. The organic phases and any aqueous phases that contained >5% of the applied were then concentrated under reduced pressure at 30°C, and aliquots of the concentrates were analyzed using LSC. The concentrated extracts from each sample were then pooled and for total radioactivity using LSC and for individual [^{14}C]compounds using HPLC and TLC.

All soil samples were extracted three times with acetonitrile:water (8:2, v:v) at room temperature (extraction method not reported; p. 24; Scheme 1, p. 58). Samples collected at and after 7 days posttreatment were Soxhlet-extracted with acetonitrile:water (8:2, v:v) for 4 hours. Aliquots of the individual extracts were analyzed for total radioactivity using LSC, then pooled. The acetonitrile was removed from the pooled extracts using a rotary evaporator and the resulting aqueous solutions were mixed with 20% acetonitrile; aliquots were analyzed using LSC. The extracts were partitioned once with ethyl acetate; aliquots of the aqueous and organic phases were analyzed using LSC. The organic phases and any aqueous phases that contained >5% of the applied were then concentrated under reduced pressure at 30°C, and aliquots of the concentrates were analyzed using LSC. The concentrated extracts from each sample were then

pooled and analyzed for total radioactivity using LSC and for individual [^{14}C]compounds using HPLC and TLC.

Soil samples from 100 days posttreatment were further extracted (harsh extraction) by refluxing for *ca.* 4 hours with acetonitrile:1.0N HCl (1:1, v:v; p. 25; Scheme 1, p. 58). The resulting extracts were analyzed using LSC.

Nonextractable residue determination: The extracted soil was air-dried and homogenized, and subsamples were combusted and analyzed for total radioactivity using LSC (pp. 24-25 Scheme 1, p. 58). Oxidation efficiency was >95%.

To separate nonextractable [^{14}C]residues into humin, humic acid, and fulvic acid, aliquots of the soils from day 100 were extracted by shaking under reflux conditions with acetonitrile:1.0N HCl (1:1, v:v) for *ca.* 4 hours (p. 25; Scheme 2, p. 59). Aliquots of the extracts were analyzed for total radioactivity using LSC. The extracts were then shaken with 0.5N NaOH for *ca.* 16 hours, centrifuged, and extracted a second time with 0.5N NaOH for *ca.* 30 minutes followed by centrifugation. The soils were then washed with water, centrifuged, and the water was decanted and added to the previous extracts. The pooled extracts were reduced to a pH of *ca.* 1, and the samples were centrifuged. The resulting supernatant (fulvic acid) was decanted and analyzed for total radioactivity using LSC. The remaining solid (humic acid) was combusted and analyzed using LSC. The remaining solid after the water wash (humin) was combusted and analyzed using LSC.

Volatile residue determination: Aliquots of the trapping solutions were analyzed for total radioactivity using LSC (pp. 23, 26). [^{14}C]Residues in the NaOH trapping solutions at 22 and 56 days were determined to be CO_2 by precipitation with barium hydroxide.

Total ^{14}C measurement: Total [^{14}C]residues were determined by summing the concentrations of residues remaining in the soil extracts, extracted soil, and volatile trapping solutions (Tables 7-8, pp. 47-48).

Derivatization method, if used: A derivatization method was not employed.

Identification and quantification of parent compound: Aliquots of the soil and water extracts were analyzed using HPLC under the following conditions (pp. 26-27): Hypersil ODS column (25 cm H 4.6 mm; 5 Φm particle size), gradient mobile phase combining (A) water, (B) acetonitrile, and (C) 0.02M dipotassiumhydrogenphosphate and 0.02M potassiumdihydrogenphosphate (2:3, v:v) in water adjusted to pH 6.7 [percent A:B:C (v:v:v) at 0 minutes, 50:30:20; 5 minutes, 30:50:20; 20-25 minutes, 0:80:20; 25.1-30 minutes, 50:30:20], flow rate of 1.5 mL/minute, with UV (254 nm) detection. The eluant was continuously collected (1.5 mL units) and analyzed using LSC. [^{14}C]Oxyfluorfen was identified by comparison to the retention time of an unlabeled reference standard of oxyfluorfen (Lot Number DAC-22-96-B; purity 99.8%; p. 17, Figures 11-14, pp. 71-74).

One- and two-dimensional TLC were used to confirm HPLC data using pre-coated plates (5 H 20 cm and 20 H 20 cm; 0.25 mm thickness) of silica gel 60 F_{254} (normal phase) or RP-18 (reverse phase) developed in the following solvent systems: (SS 4) hexane:ethyl acetate:acetic acid (50:20:0.5, v:v:v), (SS 5) chloroform:methanol:formic acid:water (60:30:4:2, v:v:v:v), (SS 7) methanol, (SS 10) ethyl acetate:methanol (1:1, v:v), (SS 11) acetonitrile:water:acetic acid (10:10:4, v:v:v), (SS 12) acetonitrile:water:acetic acid (90:10:1, v:v:v), or (SS 13) ethyl acetate (p. 27). The samples were visualized using UV (254 nm) and submitted to phosphor imaging to confirm HPLC results.

Identification and quantification of transformation products: Transformation products were separated and quantified using HPLC and TLC as described for the parent compound. No reference compounds were used.

Detection limits (LOD, LOQ) for the parent compound: Limits of Detection (LOD) and Limits of Quantification (LOQ) for LSC analysis were 2H (40 dpm) and 3H (60 dpm) the background radioactivity, respectively (p. 29). For HPLC analysis, the LOD and LOQ were 200 dpm (p. 30; Appendix I, Figure AI-1, p. 85).

Detection limits (LOD, LOQ) for the transformation products: The LOD and LOQ were the same as reported for the parent compound.

II. RESULTS AND DISCUSSION:

A. TEST CONDITIONS: The incubation temperature (20 ∀ 2EC) was maintained throughout the experiment; no supporting data were provided. The pH of the river water averaged 8.27 ∀ 0.21 and of the pond water averaged 8.15 ∀ 0.11 (pp. 33-34; Tables 5-6, pp. 45-46). Redox potentials in the **river water** were 172 mV at the time of treatment and ranged from 175 to 220 mV throughout the study (Table 5, p. 45). The oxygen concentration of the water averaged 6.5 ± 1.1 mg/L. Redox potentials in the sediment layer were -128 mV at the time of treatment and ranged from -98 to -161 mV throughout the study. Redox potentials in the **pond water** were 201 mV at the time of treatment and ranged from 157 to 322 mV throughout the study (Table 6, p. 46). The oxygen concentration of the water averaged 6.0 ± 0.9 mg/L. Redox potentials in the sediment layer were -103 mV at the time of treatment and ranged from -73 to -151 mV throughout the study.

B. MATERIAL BALANCE: Overall recoveries of [^{14}C]residues averaged 93.9 ∀ 3.6% (n = 18; range 86.4-100.8%) of the applied from the river system and 94.9 ∀ 2.7% (n = 18; 90.9-101.6%) from the pond system (Tables 7-8, pp. 47-48). The ratio of [^{14}C]residues in the water and sediment were *ca.* 2:1 (v:w) at 0.25 days posttreatment, 1:1 at 2 days, 1:4 at 7 days, and 1:10 at 56 days.

Table 6a: Biotransformation of [^{14}C]oxyfluorfen, expressed as percentage of applied radioactivity (n = 2, mean ± s.d.), in river water/sandy loam sediment system under anaerobic conditions.

Compound		Sampling times (days)								
		0	0.25 [1]	1	2	7	14	28	56	100
Oxyfluorfen	Water	62.2 ∀ 0.2	68.6 ∀ 3.3	55.3 ∀ 1.2	44.6 ∀ 3.2	15.8 ∀ 0.8	19.8 ∀ 4.5	4.0 ∀ 3.3	1.1 ∀ 0.4	<0.3 [2]
	Sediment	32.6 ∀ 0.1	29.8 ∀ 1.0	37.7 ∀ 1.6	50.2 ∀ 3.4	70.5 ∀ 7.8	65.7 ∀ 3.3	43.2 ∀ 13.2	32.9 ∀ 4.9	25.2 ∀ 5.2
	System	94.7 ∀ 0.3	98.4 ∀ 2.3	93.0 ∀ 0.4	94.8 ∀ 0.2	86.3 ∀ 7.0	85.5 ∀ 1.2	47.2 ∀ 16.4	34.0 ∀ 5.4	25.3 ± 5.4
M2	Water	ND	ND	ND	ND	ND	ND	<1.5	1.1 ∀ 0.3	1.8 ∀ 0.1
	Sediment	ND	ND	ND	ND	ND	ND	ND	ND	ND
	System	ND	ND	ND	ND	ND	ND	<1.5	1.1 ∀ 0.3	1.8 ∀ 0.1
M3	Water	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Sediment	ND	ND	ND	ND	ND	ND	<1.5	1.9 ∀ 0.9	<1.3
	System	ND	ND	ND	ND	ND	ND	<1.5	1.9 ∀ 0.9	<1.3
M5	Water	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Sediment	ND	ND	ND	ND	ND	ND	<9.6	4.9 ∀ 0.4	3.7 ∀ 2.4
	System	ND	ND	ND	ND	ND	ND	<9.6	4.9 ∀ 0.4	3.7 ∀ 2.4
M6	Water	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Sediment	ND	ND	ND	ND	ND	ND	<4.6	1.9 ∀ 0.5	2.0 ∀ 1.1
	System	ND	ND	ND	ND	ND	ND	<4.6	1.9 ∀ 0.5	2.0 ∀ 1.1
M7	Water	ND	ND	ND	ND	ND	ND	ND	<0.4	<0.1
	Sediment	ND	ND	ND	ND	ND	ND	ND	1.6 ∀ 0.7	ND
	System	ND	ND	ND	ND	ND	ND	ND	<1.8	<0.1

Compound		Sampling times (days)								
		0	0.25 [1]	1	2	7	14	28	56	100
M8	Water	ND	ND	ND	ND	ND	ND	ND	<0.3	<0.1
	Sediment	ND	ND	ND	ND	ND	ND	ND	<1.6	<0.6
	System	ND	ND	ND	ND	ND	ND	ND	<1.0	<0.4
CO_2		NP	<0.1 ∀ 0.0	<0.1	0.2 ∀ 0.1	0.5 ∀ 0.1	1.0 ∀ 0.3	4.7 ∀ 1.1	7.9 ∀ 0.1	9.0 ∀ 0.2
Volatile organics		NP	<0.1 ∀ 0.0	<0.1 ∀ 0.0	<0.1	0.1 ∀ 0.0	0.5 ∀ 0.1	0.3 ∀ 0.1	0.4 ∀ 0.1	0.5 ∀ 0.3
Total extractable residues [3]		32.6 ∀ 0.1	29.8 ∀ 1.0	37.7 ∀ 1.6	50.2 ∀ 3.4	70.6 ∀ 7.7	65.8 ∀ 3.2	51.1 ∀ 2.1	43.9 ∀ 3.2	31.8 ∀ 1.1
Nonextractable residues		0.8 ∀ 0.1	0.7 ∀ 0.0	1.3 ∀ 0.4	2.0 ∀ 0.4	4.5 ∀ 0.0	7.5 ∀ 0.4	30.4 ∀ 2.2	38.7 ∀ 4.2	45.6 ∀ 3.3
Total recovery		95.5 ∀ 0.2	99.1 ∀ 2.4	94.4 ∀ 0.6	96.9 ∀ 0.7	91.3 ∀ 6.9	94.5 ∀ 0.8	91.2 ∀ 1.2	93.3 ∀ 0.6	89.0 ∀ 2.1

Data were obtained from Table 7, p. 47 and Tables 9-11, pp. 49-51 of the study report. Means and standard deviations were reviewer-calculated; values differed slightly from those reported by the study author due to rounding (See DER Attachment 2).

1 The 0.25-day sample was treated separate from the rest of the samples in the set. No explanation was provided.

2 Single values with a < sign indicate that the compound was not detected in one of the replicate samples.

3 Total extractable residues are the sum of the room temperature and Soxhlet extractions with acetonitrile:water (8:2, v:v).

ND = Not detected, limit of quantification 200 dpm.

NP = Not performed.

Table 6b: Biotransformation of [^{14}C]oxyfluorfen, expressed as percentage of applied radioactivity (n = 2, mean ± s.d.), in pond water/silt loam sediment system under anaerobic conditions.

Compound		Sampling times (days)								
		0	**0.25** [1]	**1**	**2**	**7**	**14**	**28**	**56**	**100**
Oxyfluorfen	Water	56.7 ∀ 0.5	71.4 ∀ 0.1	53.9 ∀ 5.9	46.4 ∀ 4.2	16.9 ∀ 0.8	5.9 ∀ 2.6	5.2 ∀ 2.5	2.6 ∀ 2.5	NA
	Sediment	36.2 ∀ 3.3	27.6 ∀ 2.4	40.7 ∀ 5.9	46.4 ∀ 3.9	68.1 ∀ 1.6	63.9 ∀ 4.6	46.1 ∀ 14.4	23.0 ∀ 5.9	7.9 ∀ 4.4
	System	92.8 ∀ 2.8	99.0 ∀ 2.5	94.6 ∀ 0.1	92.8 ∀ 0.4	85.0 ∀ 0.7	69.7 ∀ 7.2	51.2 ∀ 11.9	25.6 ∀ 8.4	7.9 ∀ 4.4
M1	Water	ND	ND	ND	ND	ND	<3.5 [2]	ND	ND	NA
	Sediment	ND	ND	ND	ND	ND	ND	ND	ND	ND
	System	ND	ND	ND	ND	ND	<3.5	ND	ND	ND
M2	Water	ND	ND	ND	ND	ND	<0.7	<3.0	1.0 ∀ 0.1	NA
	Sediment	ND	ND	ND	ND	ND	ND	ND	ND	ND
	System	ND	ND	ND	ND	ND	<0.7	<3.0	1.0 ∀ 0.1	ND
M3	Water	ND	ND	ND	ND	ND	ND	ND	ND	NA
	Sediment	ND	ND	ND	ND	ND	<1.3	0.7 ∀ 0.0	<1.5	ND
	System	ND	ND	ND	ND	ND	<1.3	0.7 ∀ 0.0	<1.5	ND
M4	Water	ND	ND	ND	ND	ND	ND	ND	ND	NA
	Sediment	ND	ND	ND	ND	ND	<1.1	<0.5	ND	ND
	System	ND	ND	ND	ND	ND	<1.1	<0.5	ND	ND
M5	Water	ND	ND	ND	ND	ND	ND	ND	ND	NA
	Sediment	ND	ND	ND	ND	ND	ND	<1.3	2.5 ∀ 1.7	3.0 ∀ 2.3
	System	ND	ND	ND	ND	ND	ND	<1.3	2.5 ∀ 1.7	3.0 ∀ 2.3

Compound		Sampling times (days)								
		0	0.25 [1]	1	2	7	14	28	56	100
M6	Water	ND	ND	ND	ND	ND	ND	ND	ND	NA
	Sediment	ND	ND	ND	ND	ND	ND	1.4 ∀ 0.4	<1.7	ND
	System	ND	ND	ND	ND	ND	ND	1.4 ∀ 0.4	<1.7	ND
M7	Water	ND	ND	ND	ND	ND	ND	ND	<0.2	NA
	Sediment	ND	ND	ND	ND	ND	ND	ND	ND	ND
	System	ND	ND	ND	ND	ND	ND	ND	<0.2	ND
M9	Water	ND	ND	ND	ND	ND	ND	ND	ND	NA
	Sediment	ND	ND	ND	ND	ND	ND	ND	ND	14.1 ∀ 0.8
	System	ND	ND	ND	ND	ND	ND	ND	ND	14.1 ∀ 0.8
CO_2		NP	<0.1 ∀ 0.0	<0.1	0.3 ∀ 0.3	0.5 ∀ 0.1	0.9 ∀ 0.9	4.6 ∀ 2.0	8.0 ∀ 0.4	9.4 ∀ 1.11
Volatile organics		NP	<0.1 ∀ 0.0	<0.6	0.1 ∀ 0.0	0.3 ∀ 0.1	0.5 ∀ 0.1	0.3 ∀ 0.1	0.6 ∀ 0.1	0.8 ∀ 0.5
Total extractable residues [3]		36.2 ∀ 3.3	27.6 ∀ 2.3	40.7 ∀ 5.9	46.4 ∀ 3.9	68.1 ∀ 1.6	65.1 ∀ 2.9	49.0 ∀ 14.6	27.1 ∀ 1.9	24.9 ∀ 1.3
Nonextractable residues		1.3 ∀ 0.0	0.9 ∀ 0.2	2.1 ∀ 0.1	2.6 ∀ 0.3	9.5 ∀ 0.6	18.1 ∀ 2.9	32.4 ∀ 7.8	52.3 ∀ 3.6	59.3 ∀ 0.7
Total recovery		94.1 ∀ 2.8	99.8 ∀ 2.6	97.0 ∀ 0.1	95.8 ∀ 0.2	95.3 ∀ 0.1	92.5 ∀ 1.2	92.9 ∀ 0.3	91.6 ∀ 0.9	95.6 ∀ 2.8

Data were obtained from Table 8, p. 48 and Tables 12-14, pp. 52-54 of the study report. Means and standard deviations were reviewer-calculated; values differed slightly from those reported by the study author due to rounding (See DER Attachment 2).

1 The 0.25-day sample was treated separate from the rest of the samples in the set. No explanation was provided.

2 Single values with a < sign indicate that the compound was not detected in one of the replicate samples.

3 Total extractable residues are the sum of the room temperature and Soxhlet extractions with acetonitrile:water (8:2, v:v).

ND = Not detected, limit of quantification 200 dpm.

NP = Not performed.

NA = Not analyzed.

C. TRANSFORMATION OF PARENT COMPOUND: In the total river system (water plus sediment), [^{14}C]oxyfluorfen varied from an average of 93.0 to 98.4% of the applied at 0 through 2 days posttreatment with no pattern of decline, then decreased to 85.5-86.3% at 7 and 14 days, 47.2% at 28 days, and 25.3% % at 100 days (study termination, Table 11, p. 51). In the water, [^{14}C]oxyfluorfen averaged 62.2-68.6% of the applied at 0-0.25 days posttreatment, then decreased to 15.8-19.8% at 7 and 14 days, 4.0% at 28 days and <0.3% at 100 days (Table 9, p. 49). In the sediment, [^{14}C]oxyfluorfen increased to a maximum average of 70.5% of the applied at 7 days posttreatment, then decreased to 32.9% at 56 days and 25.2% at 100 days (Table 10, p. 50).

In the total pond total system, [^{14}C]oxyfluorfen varied from an average of 92.8 to 99.0% at 0 through 2 days posttreatment with no pattern of decline, then decreased to 85.0% at 7 days, 51.2% at 28 days, 25.6% at 56 days, and 7.9% at 100 days (study termination, Table 14, p. 54). In the water, [^{14}C]oxyfluorfen averaged 53.9-71.4% of the applied at 0-1 day posttreatment, then decreased to 16.9% at 7 days, 5.9% at 14 days and 2.6% at 56 days (last interval analyzed; Table 12, p. 52). In the sediment, [^{14}C]oxyfluorfen increased to a maximum average of 68.1% of the applied at 7 days posttreatment, then decreased to 23.0% at 56 days and 7.9% at 100 days (Table 13, p. 53).

Half-Life/DT50/DT90: Based on first-order linear regression analysis, oxyfluorfen dissipated with a reviewer-calculated half-life of 47 days in the total river system and 27 days in the total pond system (DER Attachment 2). Reviewer-calculated nonlinear (single, 2 parameter) half-lives for oxyfluorfen in the total river and pond systems were 40 and 30 days, respectively. In both systems, the observed DT50 was *ca.* 28 days.

In the river system, oxyfluorfen dissipated with a linear half-life of 11.6 days in the water and 61.9 days in the sediment (DER Attachment 2). Nonlinear half-lives were 4.7 and 50.6 days in the water and sediment, respectively. Observed DT50 values were <7 and 56 days for the water and sediment.

In the pond system, oxyfluorfen dissipated with a linear half-life of 10.8 days in the water and 28.3 days in the sediment (DER Attachment 2). Nonlinear half-lives were 3.9 and 31.5 days in the water and sediment, respectively. Observed DT50 values were <7 and <56 days for the water and sediment.

DT50 values for [^{14}C]oxyfluorfen were determined by the study author based on first-order nonlinear degradation kinetics analysis using the Origin program (v. 3.5; pp. 31-32). For the river system, the calculated DT50 values for [^{14}C]oxyfluorfen were 3.5, 50.6, and 39.6 days for the water, sediment, and total system, respectively (pp. 36-37; Figures 7-9, pp. 67-69). For the pond system, the calculated DT50 values for [^{14}C]oxyfluorfen were 3.9, 31.5, and 29.6 days for the water, sediment, and total system, respectively.

Half-lives/DT50/DT90 for the dissipation of [^{14}C]oxyfluorfen

Soil type	First order linear			DT50 (days)	DT90 (days)
	Half-life/DT50 (days)	Regression equation	r^2		
River water/sediment					
Linear/natural log					
Water	11.6	y = -0.0599x + 3.7615	0.9222	--	--
Sediment	61.9	y = -0.0112x + 4.2336	0.8131	--	--
Total system	47.2	y = -0.0147x + 4.5285	0.8815	--	--
Nonlinear/normal					
Water	4.7	--	0.9538	3.5	11.6
Sediment	50.6	--	0.9792	50.6	168.2
Total system	39.6	--	0.9248	39.6	131.5
Observed DT50					
Water	<7	--	--	--	--
Sediment	*ca.* 56	--	--	--	--
Total system	*ca.* 28	--	--	--	--
Pond water/sediment					
Linear/natural log					
Water	10.8	y = -0.0642x + 3.7268	0.7686	--	--
Sediment	28.3	y = -0.0245x + 4.4627	0.9286	--	--
Total system	26.9	y = -0.0256x + 4.5941	0.9573	--	--
Nonlinear/normal					
Water	3.9	--	0.9584	3.9	13.1
Sediment	31.5	--	0.9858	31.5	104.6
Total system	29.6	--	0.9797	29.6	98.4
Observed DT50					
Water	<7	--	--	--	--
Sediment	<56	--	--	--	--
Total system	*ca.* 28	--	--	--	--

Half-life values were calculated by the reviewer using data obtained from Tables 9-14, pp. 49-54 of the study report. DT50 and DT90 values were calculated by the study author using Origin. Data obtained from pp. 31-32, 36-37 and Figures 7-9, pp. 67-69 of the study report.

TRANSFORMATION PRODUCTS: No major transformation products were isolated from any of the test soils at any time during the study (Tables 9-14, pp. 49-54). Six minor

transformation products (M2, M3, M5, M6, M7, M8) were isolated from the river system and eight (M1, M2, M3, M4, M5, M6, M7, M9) were isolated from the pond system, these compounds were not identified. These compounds were not detected until 14 days posttreatment and each averaged ≤4.9% of the applied through 100 days with one exception. M5 was 9.6% of the applied in one river water sample at 28 days posttreatment; M5 was not detected in the replicate sample from this interval and averaged 3.7% at 100 days.

NONEXTRACTABLE AND EXTRACTABLE RESIDUES: In the river sediment, total extractable [^{14}C]residues increased to a maximum average of 70.6% of the applied at 7 days posttreatment, then declined to 31.8% at 100 days (study termination; Table 7, p. 47). Nonextractable [^{14}C]residues increased to a maximum average of 45.6% of the applied at 100 days posttreatment. Harsh extraction of the 100-day extracted sediment released an additional 6.8-7.1% of the applied; TLC analysis of this extract yielded at least two very polar compounds that were not further characterized (Table 17, p. 57; p. 36, Figure 22, p. 82). Fractionation of the nonextracted residues in the 100-day harsh-extracted soil (36.2-41.0% of the applied) determined that 2.3-2.5%, 0.6-0.7%, and 33.3-37.8% of the applied was associated with fulvic acids, humic acids, and humin, respectively.

In the pond sediment, total extractable [^{14}C]residues increased to a maximum average of 68.1% of the applied at 7 days posttreatment, then declined to 24.9% at 100 days (study termination; Table 8, p. 48). Nonextractable [^{14}C]residues increased to a maximum average of 59.3% of the applied at 100 days. Harsh extraction of the 100-day extracted sediment released an additional 15.5-17.2% of the applied; TLC analysis of this extract yielded at least two very polar compounds that were not further characterized (Table 17, p. 57; p. 36, Figure 22, p. 82). Fractionation of the nonextracted residues in the 100-day harsh-extracted soil (42.6-43.3% of the applied) determined that 1.7-2.0%, 2.7-2.8%, and 38.2-38.5% of the applied was associated with fulvic acids, humic acids, and humin, respectively.

VOLATILIZATION: At study termination (100 days), $^{14}CO_2$ and volatile organic [^{14}C]residues totaled an average 9.0% and 0.5% of the applied, respectively, in the river system and 9.4% and 0.8%, respectively, in the pond system (Tables 7-8, pp. 47-48).

TRANSFORMATION PATHWAY: A transformation pathway was provided by the study author (pp. 37, 39; Figure 23, p. 83). Oxyfluorfen applied to water dissipates rapidly by mineralization to CO_2 and minor transformation products and by incorporated into the organic matter of the sediment.

Table 7: Chemical names and CAS numbers for the transformation products of oxyfluorfen.

Applicants Code Name	CAS Number	Chemical Name	Chemical Formula	Molecular Weight (g/mol)	Smiles String
M1	--	--	--	--	--
M2	--	--	--	--	--
M3	--	--	--	--	--
M4	--	--	--	--	--
M5	--	--	--	--	--
M6	--	--	--	--	--
M7	--	--	--	--	--
M8	--	--	--	--	--
M9	--	--	--	--	--

D. SUPPLEMENTARY STUDY- RESULTS: No supplemental experiments were reported.

III. STUDY DEFICIENCIES

1. It was not established that the soils used in this study were comparable to soils that would be found at the intended use sites in the United States. The soils used in this study were from Switzerland and the FAO classification was not provided.

2. A soil from the US was not included in the study.

IV. REVIEWER'S COMMENTS

1. The 0.25-day sample was treated separately, and the study author did not provide any information as to when this sample was treated in relation to the remaining sample. Overall recovery of [^{14}C]residues and oxyfluorfen is higher from this sample than from other samples in the experiment. The study author did not provide any explanation as to why this sample was separate. The results from this sample do not affect the interpretation of the study results.

2. At 100 days posttreatment, the pond water contained #1.7% of the applied radioactivity (p. 38; Table 12, p. 52). This fraction was referred to as "non-recovered" and was not analyzed by HPLC or TLC.

3. The study author reported water:sediment ratios of 4:1 for the river system and 8:1 for the pond system (p. 20). The reviewer could only approximate these values. Both systems consisted of 550 mL water to 220 g wet sediment (2.5:1). It was presumed that the 550 mL of water did not include the water associated with the sediment. Therefore for the river system, this translated to 137 g dry sediment, 83 mL of water associated with the sediment, and 550 mL water (sediment:total water, 4.6:1). For the pond system, this translated to 84 g dry sediment, 136 mL water associated with the sediment, and 550 mL water (sediment:water, 8.2:1).

4. The vapor pressure/volatility, UV absorption, pKa, and K_{ow}/log K_{ow} of oxyfluorfen were not reported. In addition, a physical description (color, form) of oxyfluorfen was not reported.

5. The soil and water collection procedures were not provided and a pesticide use history at the collection site was not reported.

6. HPLC chromatograms of the water phases and soil extracts are presented in Figures 11-14, pp. 71-74 and Figures 17-18, pp. 77-78 of the study report. TLC chromatograms of the water phases and soil extracts are presented in Figures 15-16, pp. 75-76 and Figures 19-22, pp. 79-82 of the study report.

7. The study author reported that the maximum field application rate for oxyfluorfen was 1440 g a.i./ha (p. 21). The nominal application rate used in this study was 0.480 mg a.i./L, which is equivalent to a field rate of 1440 g a.i./ha assuming that the water surface is equivalent to the soil surface and that there is a homogeneous distribution of oxyfluorfen in the top 30 cm of the water column.

V. REFERENCES:

1. U.S. Environmental Protection Agency. 1982. Pesticide Assessment Guidelines, Subdivision N, Chemistry: Environmental Fate, Section 162-4, Aerobic Aquatic Metabolism Studies. Office of Pesticide and Toxic Substances, Washington, DC. EPA 540/9-82-021.

2. U.S. Environmental Protection Agency. 1989. FIFRA Accelerated Reregistration, Phase 3 Technical Guidance. Office of the Prevention, Pesticides, and Toxic Substances, Washington, DC. EPA 540/09-90-078.

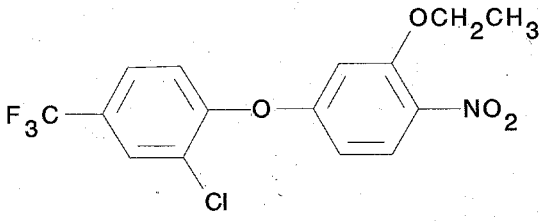
3. U.S. Environmental Protection Agency. 1993. Pesticide Registration Rejection Rate Analysis - Environmental Fate. Office of the Prevention, Pesticides, and Toxic Substances, Washington, DC. EPA 738-R-93-010.

Attachment 1: Structures of Parent Compound and Transformation Products

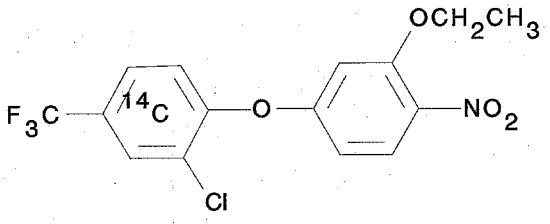
Oxyfluorfen [RH-2915; Goal]

IUPAC Name:	2-Chloro-α,α,α-trifluoro-ρ-tolyl-3-ethoxy-4-nitrophenyl ether.
CAS Name:	2-Chloro-1-(3-ethoxy-4-nitrophenoxy)-4-(trifluoromethyl)benzene.
CAS No.:	42874-03-3.
SMILES String:	FC(c1ccc(c(c1)Cl)Oc1ccc(c(c1)OCC)N(=O)=O)(F)F (ISIS v2.3/Universal SMILES). Clc1cc(C(F)(F)F)ccc1Oc2cc(OCC)c(N(=O)(=O))cc2 (EPI Suite, v3.12).

Unlabeled



[Chlorophenyl ring-UL-^{14}C]oxyfluorfen



^{14}C = position of radiolabel.

Identified Compounds

Oxyfluorfen [RH-2915; Goal]

IUPAC Name: 2-Chloro-α,α,α-trifluoro-ρ-tolyl-3-ethoxy-4-nitrophenyl ether.
CAS Name: 2-Chloro-1-(3-ethoxy-4-nitrophenoxy)-4-(trifluoromethyl)benzene.
CAS No.: 42874-03-3.
SMILES String: FC(c1ccc(c(c1)Cl)Oc1ccc(c(c1)OCC)N(=O)=O)(F)F
(ISIS v2.3/Universal SMILES).
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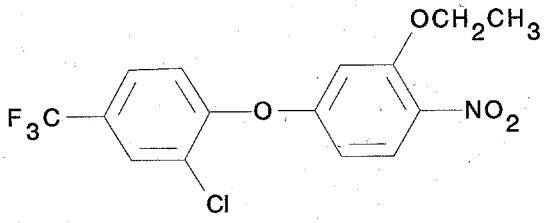
(EPI Suite, v3.12).



Carbon Dioxide

IUPAC Name: Not reported.
CAS Name: Not reported.
CAS Number: Not reported.